Magnetic Inelastic X-ray Scattering as a Probe of Electronic Excitations in Correlated Electron Materials

Pedro A. Montano[a], Yinwan Li[b,c], J. F. Mitchell[c], B. Barbiellini[d], P. E. Mijnarends [d,e], S. Kaprzyk[d,f], A. Bansil[d], *[a] SUFD, U. S. Department of Energy, 1000 Independence Avenue, Washington DC 20585, USA. [b]Department of Physics, University of Illinois, Chicago IL 60680. [c]Materials Science Division, Argonne National Laboratory, Argonne IL 60439. [d]Physics Department, Northeastern University, Boston MA 02115. [e]Department of Radiation, Radionuclides & Reactors, Faculty of Applied Sciences, Delft University of Technology, Delft, The Netherlands. [f]Academy of Mining and Metallurgy AGH, 30059 Krakow, Poland.* E-mail: pedro.montano@science.doe.gov

The magnetic x-ray scattering technique in the deeply inelastic (Compton) regime is emerging as a powerful new spectroscopic window for understanding the properties of magnetic electrons in complex materials. Here we consider results on three correlated electron systems of current interest: The double layer manganite $La_{1.2}Sr_{1.8}Mn_2O_7$, the perovskite manganite $La_{0.7}Sr_{0.3}MnO_3$ and the magnetite F_3O_4. First principles band theory computations using the conventional local density approximation (LDA) as well as computations going beyond the LDA framework for treating correlation effects are used to gain insight into recent magnetic Compton scattering measurements. We show how in the double layer manganite the [110] magnetic Compton profile (MCP) contains a distinct signature of the d-electrons of x^2-y^2 symmetry, allowing us to monitor significant changes in the occupancy of these orbitals as a function of temperature over the range of 5-200K. An itinerant electron contribution is suggested at all temperatures in magnetite. In magnetite, we find that the magnetic moment associated with unpaired spins is non-integral and we adduce that the charge ordering model of the Verwey transition is not tenable.

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